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Title:	Midterm Report: Data Driven Modeling of Non-Equilibrium Dynamics in Chemical and Materials Systems
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Midterm Report: Data Driven Modeling of Non-Equilibrium Dynamics in Chemical and Materials Systems

Ben Nebgen

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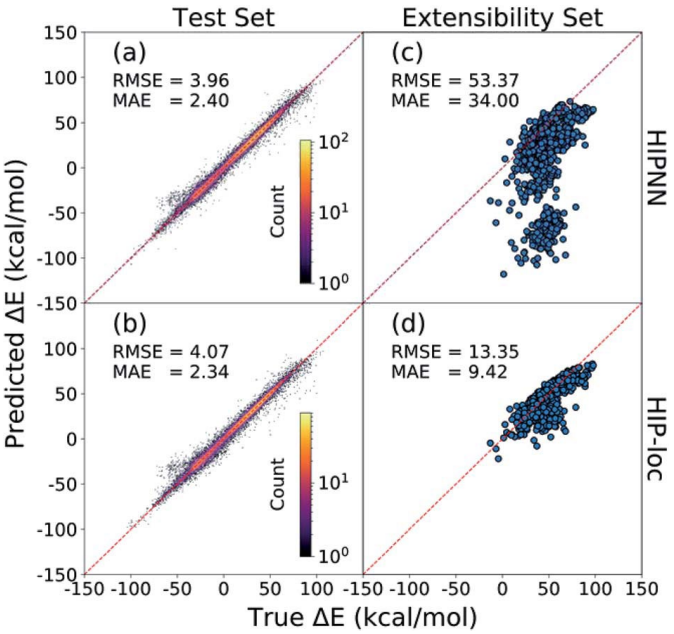
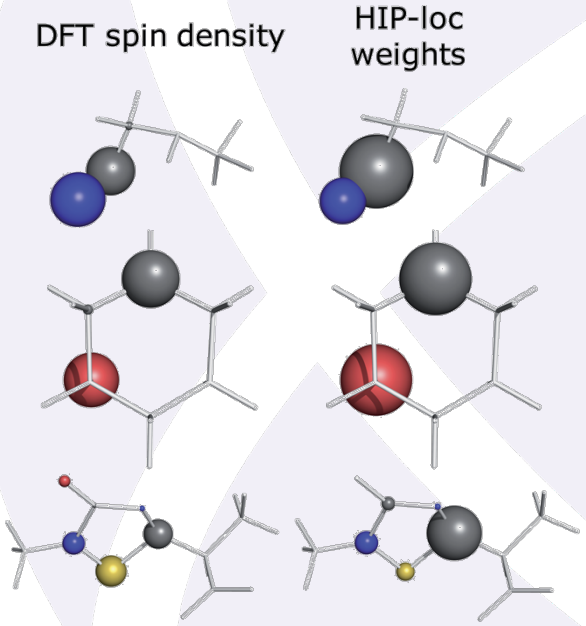
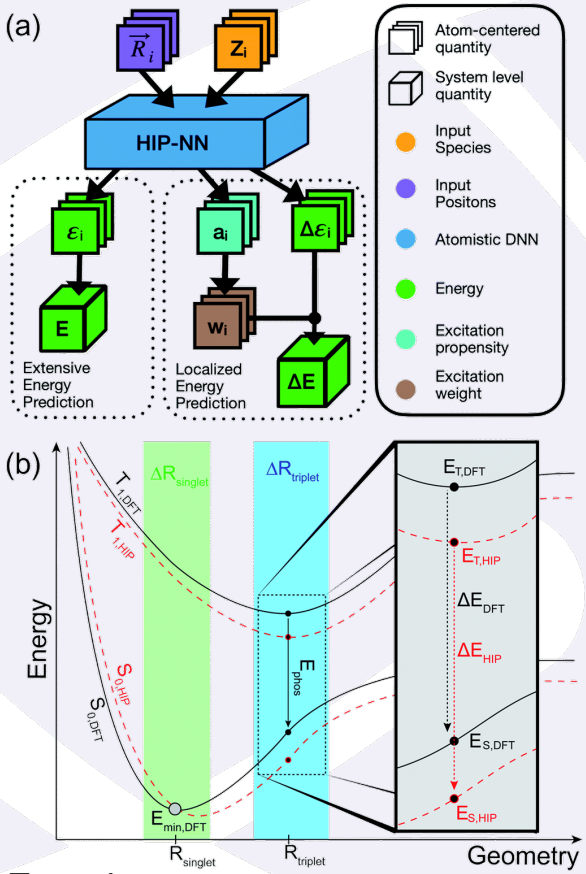
Predicting Phosphorescence Energies with ML

- Data from quantum mechanical calculations were generated to train a NN model for predicting phosphorescence energies (left).
- Model uses localization layer, which learns to resemble the triplet spin density without explicit training.





HIPPYNN model for predicting phosphorescence energy gaps.



Sifain Et al. *Chem. Sci.* **12**, 10207-10217 (2021).
Corresponding Dataset: "Dataset of Singlet and Triplet Energies and Forces for Organic Molecules": LA-UR-21-25454

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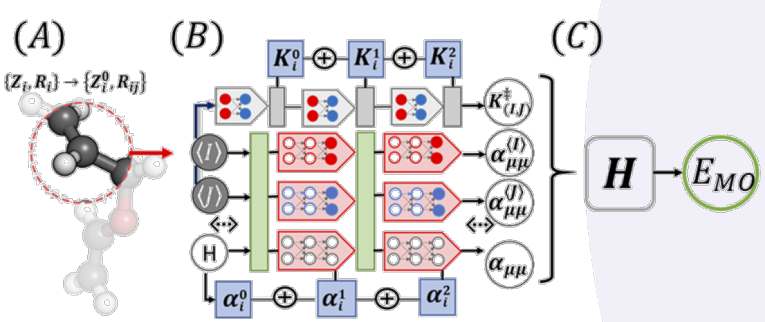
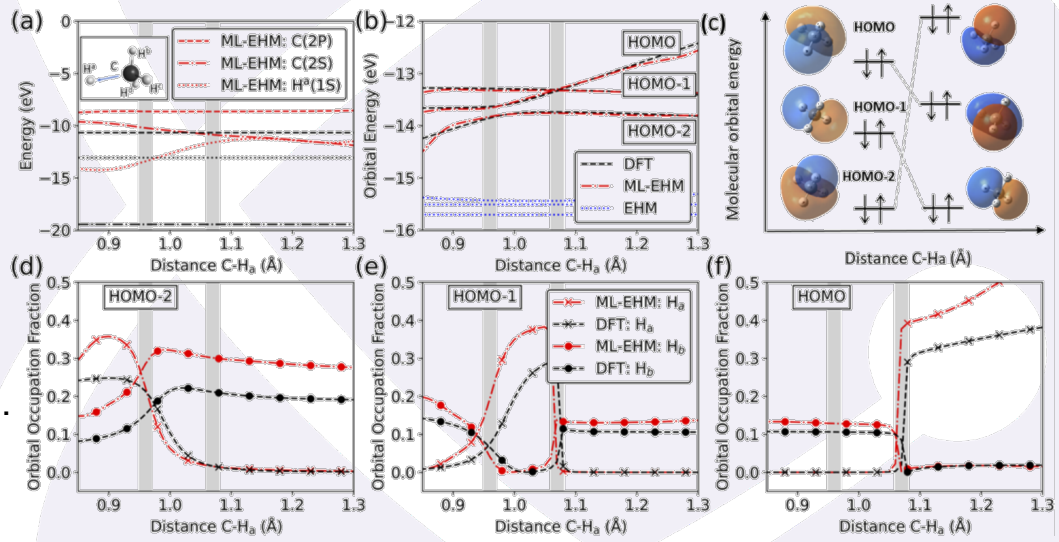
Hückel model for Predicting Molecular Orbital Properties

- HIPPYNN can be used to dynamically parameterize and Hückel theory Hamiltonian.
- The resultant model is in extremely close agreement to more computationally expensive quantum methods (bottom right).

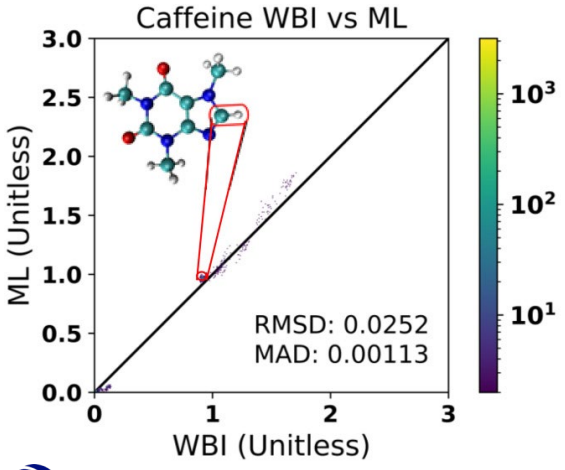


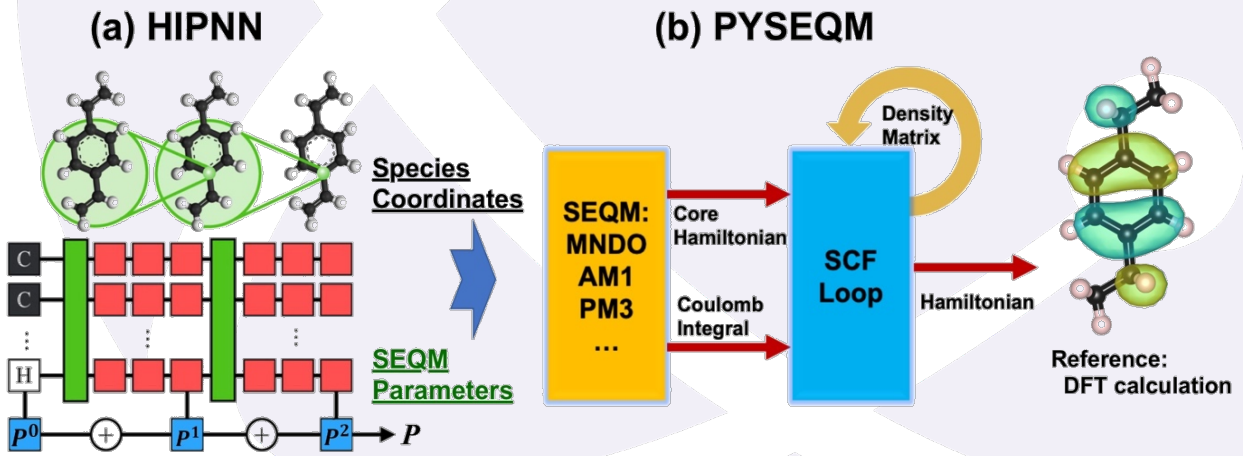


Zubatiuk Et al. *J. Chem. Phys.* **154**, 244108 (2021).
Corresponding Dataset: "Dataset of Molecular Orbital Energies and Densities for Organic Molecules": LA-UR-21-23368

Release of HIPPYNN Software

- As part of this allocation, the HIPPYNN software package was tested and openly released though the Feynman Center for Innovation.
- HIPPYNN is a Neural Network for learning chemical and material properties of atomistic systems.
- Advanced applications of this neural network are determining bond orders (bottom left), parameterizing quantum Hamiltonians (bottom right), and modeling phosphorescence energies (previous slide).
- Download from: https://github.com/lanl/hippynn





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Public Releases

- Publications
  - Zubatyuk, R.; Smith, J. S.; Nebgen, B.; Tretiak, S.; Isayev, O. “Teaching a neural network to attach and detach electrons from molecules” *Nat. Comm.* **12**, 4870 (2021)
  - Kulichenko, M.; Smith, J. S.; Nebgen, B.; Wai Li, Y.; Fedik, N.; Boldyrev, A. I.; Lubbers, N.; Barros, K.; Tretiak, S. “The Rise of Neural Networks for Materials and Chemical Dynamics” *J. Chem. Phys. Lett.* **12**, 26, 6227-6243 (2021).
  - Zubatiuk, T.; Nebgen, B.; Lubbers, N.; Smith, J. S.; Zubatyuk, R.; Zhou, G.; Koh, C.; Barros, K.; Isayev, O.; Tretiak, S. “Machine learned Hückel theory: Interfacing physics and deep neural networks” *J. Chem. Phys.* **154**, 244108 (2021).
  - Magedov, S.; Koh, C.; Malone, W.; Lubbers, N.; Nebgen, B. “Bond order predictions using deep neural networks” J. App. Phys. **129**, 064701 (2021).
  - Sifain, A. E.; Lystrom, L.; Messerly, R.; Smith, J. S.; Nebgen, B.; Barros, K.; Tretiak, S.; Lubbers, N.; Gifford, B. J. “Predicting phosphorescence energies and inferring wavefunction localization with machine learning” *Chem. Sci.* **12**, 10207-10217 (2021).
- Code:
  - HIPPYNN: https://github.com/lanl/hippynn
- Datasets:
  - “Dataset of energies and forces on tin configurations for machine learned interatomic potentials”: LA-UR-21-31241
  - “Dataset of Molecular Orbital Energies and Densities for Organic Molecules”: LA-UR-21-23368
  - “Dataset of Singlet and Triplet Energies and Forces for Organic Molecules”: LA-UR-21-25454
  - “Dataset of Bond Orders for Organic Molecules”: LA-UR-20-30152